Multivariate Normal Distribution II

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July 20, 2025

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Detour: Inverse of partioned symmetric matrix [1]

Consider an $n \times n$ symmetric matrix A and divide it into four blocks

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{12}^T & A_{22} \end{bmatrix}$$

For example, let $n = 3$, we have

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 5 & 6 \\ 3 & 6 & 8 \end{bmatrix}$$

We could for example have

$$A_{11} = \begin{bmatrix} 1 & 2 \\ 2 & 5 \end{bmatrix} \text{ and } A_{12} = \begin{bmatrix} 3 \\ 6 \end{bmatrix} \text{ and } A_{22} = \begin{bmatrix} 8 \end{bmatrix}$$

[1] Courtesy: http://fourier.eng.hmc.edu/e161/lectures/gaussianprocess/node6.html

Detour: Inverse of partioned symmetric matrix

Question: Write $B = A^{-1}$ in terms of the four blocks

$$B = \begin{bmatrix} B_{11} & B_{12} \\ B_{12}^T & A_{22} \end{bmatrix} = A^{-1}$$

A_{11} and $B_{11} \in R^{p \times p}$

A_{22} and $B_{22} \in R^{q \times q}$

$A_{12} = A_{21}^T$ and $B_{12} = B_{21}^T \in R^{p \times q}$

and, p + q = n

Detour: Inverse of partioned symmetric matrix

$$I_n = AA^{-1} = AB$$

$$= \begin{bmatrix} A_{11} & A_{12} \\ A_{12}^T & A_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{12}^T & B_{22} \end{bmatrix} =$$

$$\begin{bmatrix} A_{11}B_{11} + A_{12}B_{12}^T & A_{11}B_{12} + A_{12}A_{22} \\ A_{12}^T B_{11} + A_{22}B_{12}^T & A_{12}^T B_{12} + A_{22}B_{22} \end{bmatrix} = \begin{bmatrix} I_p & 0 \\ 0 & I_q \end{bmatrix}$$

Thus, we have

$$A_{11}B_{11} + A_{12}B_{12}^T = I_p$$

$$A_{11}B_{12} + A_{12}A_{22} = 0^{p \times q}$$

$$A_{12}^T B_{11} + A_{22}B_{12}^T = 0^{q \times p}$$

$$A_{12}^T B_{12} + A_{22}B_{22} = I_q$$

Detour: Inverse of partioned symmetric matrix

Moving the expressions around we get the following results.

$$B_{11} = (A_{11} - A_{12}A_{22}^{-1}A_{12}^T)^{-1} = A_{11}^{-1} + A_{11}^{-1}A_{12}(A_{22} - A_{12}^TA_{11}^{-1}A_{12})^{-1}A_{12}^TA$$

$$B_{22} = (A_{22} - A_{12}^TA_{11}^{-1}A_{12})^{-1} = A_{22}^{-1} + A_{22}^{-1}A_{12}^T(A_{11} - A_{12}A_{22}^{-1}A_{12}^T)^{-1}A_{12}A$$

$$B_{12}^T = -A_{22}^{-1}A_{12}^T(A_{11} - A_{12}A_{22}^{-1}A_{12}^T)^{-1}$$

$$B_{12}^T = -A_{11}^{-1}A_{12}^T(A_{22} - A_{12}^TA_{11}^{-1}A_{12})^{-1}$$

Determinant of Partitioned Symmetric Matrix

Theorem: Determinant of a partitioned symmetric matrix can be written as follows

$$
\begin{aligned}
|A| &= \left| \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \right| \\
&= |A_{11}||A_{22} - A_{12}^T A_{11}^{-1} A_{12}| \\
&= |A_{22}||A_{11} - A_{12} A_{22}^{-1} A_{12}^T|
\end{aligned}
$$

Determinant of Partitioned Symmetric Matrix

Proof: Note that

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} A_{11} & 0 \\ A_{12}^T & I \end{bmatrix} \begin{bmatrix} I & A_{11}^{-1} A_{12} \\ 0 & A_{22} - A_{12}^T A_{11}^{-1} A_{12} \end{bmatrix}$$
$$= \begin{bmatrix} I & A_{12} \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} A_{11} - A_{12} A_{22}^{-1} A_{12}^T & 0 \\ A_{22}^{-1} A_{21} & I \end{bmatrix}$$

The theorem is proved as we also know that

$$|AB| = |A||B|$$

and

$$\begin{vmatrix} B & 0 \\ C & D \end{vmatrix} = \begin{vmatrix} B & C \\ 0 & D \end{vmatrix} = |B| \, |D|$$

Marginalisation and Conditional of multivariate normal[2]

Assume an n-dimensional random vector

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 \end{bmatrix}$$

has a normal distribution $N(\mathbf{x}, \mu, \Sigma)$ with

$$\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \text{ and } \Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}$$

where $\mathbf{x}_1$ and $\mathbf{x}_2$ are two subvectors of respective dimensions p and q with $p + q = n$. Note that $\Sigma = \Sigma^T$, and $\Sigma_{21} = \Sigma_{21}^T$.

[2] Courtesy: http://fourier.eng.hmc.edu/e161/lectures/gaussianprocess/node7.html.

Marginalisation and Conditional of multivariate normal

Theorem:

part a: The marginal distributions of $\mathbf{x}_1$ and $\mathbf{x}_2$ are also normal with mean vector μ_i and covariance matrix Σ_{ii} $(i = 1, 2)$, respectively.

part b: The conditional distribution of $\mathbf{x}_i$ given $\mathbf{x}_j$ is also normal with mean vector

Marginalisation and Conditional of multivariate normal

Proof:

The joint density of $\mathbf{x}$ is:

$$f(\mathbf{x}) = f(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{(2\pi)^{n/2|\Sigma|^{1/2}}} exp[-\frac{1}{2}Q(\mathbf{x}_1, \mathbf{x}_2)]$$

where Q is defined as

$$Q(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x} - \mu)^T \Sigma^{-1} (\mathbf{x} - \mu)$$

$$= [(\mathbf{x}_1 - \mu_1)^T, (\mathbf{x}_2 - \mu_2)^T] \begin{bmatrix} \Sigma^{11} & \Sigma^{12} \\ \Sigma^{21} & \Sigma^{22} \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 - \mu_1 \\ \mathbf{x}_2 - \mu_2 \end{bmatrix}$$

$$= (\mathbf{x}_1 - \mu_1)^T \Sigma^{11} (\mathbf{x}_1 - \mu_1) + 2(\mathbf{x}_1 - \mu_1)^T \Sigma^{12} (\mathbf{x}_2 - \mu_2) + (\mathbf{x}_2 - \mu_2)^T \cdots$$

$$\cdots \Sigma^{22} (\mathbf{x}_2 - \mu_2)$$

Marginalisation and Conditional of multivariate normal

Here we have assumed

$$\Sigma^{-1} = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}^{-1} = \begin{bmatrix} \Sigma^{11} & \Sigma^{12} \\ \Sigma^{21} & \Sigma^{22} \end{bmatrix}$$

According to inverse of a partitioned symmetric matrix we have,

$$\Sigma^{11} = \left(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{12}^{T}\right)^{-1} = \Sigma_{11}^{-1} + \Sigma_{11}^{-1}\Sigma_{12}\left(\Sigma_{22} - A_{12}^{T}\Sigma_{11}^{T}\Sigma_{12}\right)^{-1}\Sigma$$

$$\Sigma^{22} = \left(\Sigma_{22} - \Sigma_{12}^{T}\Sigma_{11}^{-1}\Sigma_{12}\right)^{-1} = \Sigma_{22}^{-1} + \Sigma_{22}^{-1}\Sigma_{12}^{T}\left(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{12}^{T}\right)^{-1}\Sigma$$

$$\Sigma^{12} = -\Sigma_{11}^{-1}\Sigma_{12}\left(\Sigma_{22} - \Sigma_{12}^{T}\Sigma_{11}^{-1}\Sigma_{12}\right)^{-1} = \left(\Sigma^{21}\right)^{T}$$

Marginalisation and Conditional of multivariate normal

Substituting the second expression for Σ^{11}, first expression for Σ^{22}, and Σ^{12} into $Q(\mathbf{x}_1, \mathbf{x}_2)$ to get:

$$
\begin{aligned}
Q\left(\mathbf{x}_1, \mathbf{x}_2\right) = & \left(\mathbf{x}_1-\mu_1\right)^T\left[\Sigma_{11}^{-1}+\Sigma_{11}^{-1} \Sigma_{12}\left(\Sigma_{22}-A_{12}^T \Sigma_{11}^{-1} \Sigma_{12}\right)^{-1} \Sigma_{12}^T \Sigma_{11}^{-1}\right] \\
& -2\left(\mathbf{x}_1-\mu_1\right)^T\left[\Sigma_{11}^{-1} \Sigma_{12}\left(\Sigma_{22}-\Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}\right)^{-1}\right]\left(\mathbf{x}_2-\mu_2\right) \\
& +\left(\mathbf{x}_2-\mu_2\right)^T\left[\left(\Sigma_{22}-\Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}\right)^{-1}\right]\left(\mathbf{x}_2-\mu_2\right) \\
= & \left(\mathbf{x}_1-\mu_1\right)^T \Sigma_{11}^{-1}\left(\mathbf{x}_1-\mu_1\right) \\
& +\left(\mathbf{x}_1-\mu_1\right)^T \Sigma_{11}^{-1} \Sigma_{12}\left(\Sigma_{22}-A_{12}^T \Sigma_{11}^{-1} \Sigma_{12}\right)^{-1} \Sigma_{12}^T \Sigma_{11}^{-1}\right]\left(\mathbf{x}_1 -\right. \\
& -2\left(\mathbf{x}_1-\mu_1\right)^T\left[\Sigma_{11}^{-1} \Sigma_{12}\left(\Sigma_{22}-\Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}\right)^{-1}\right]\left(\mathbf{x}_2-\mu_2\right) \\
& +\left(\mathbf{x}_2-\mu_2\right)^T\left[\left(\Sigma_{22}-\Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}\right)^{-1}\right]\left(\mathbf{x}_2-\mu_2\right)
\end{aligned}
$$

Marginalisation and Conditional of multivariate normal

$$
\begin{aligned}
&= (\mathbf{x}_1 - \mu_1)^T \Sigma_{11}^{-1} \\
&\quad + \left[(\mathbf{x}_2 - \mu_2) - \Sigma_{12}^T \Sigma_{11}^{-1} (\mathbf{x}_1 - \mu_1)\right]^T \left(\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}\right)^{-1} \left[(\mathbf{x}_2 - \mu_2
\end{aligned}
$$

The last equal sign is due to the following equations for any vectors u and v and a symmetric matrix $A = A^T$:

$$
\begin{aligned}
&u^T A u - 2u^T A v + v^T A v = u^T A u - u^T A v - u^T A v + v^T A v \\
=&u^T A(u - v) - (u - v)^T A v = u^T A(u - v) - v^T A(u - v) \\
=&(u - v)^T A(u - v) = (v - u)^T A(v - u)
\end{aligned}
$$

Marginalisation and Conditional of multivariate normal

We define $b \triangleq \mu_2 + \Sigma_{12}^T \Sigma_{11}^{-1} (\mathbf{x}_1 - \mu_1)$

$$A \triangleq \Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}$$

and

$$\begin{cases} Q_1(\mathrm{x}_1) \quad \triangleq (\mathrm{x}_1 - \mu_1)^T \Sigma_1^{-1} (\mathrm{x}_1 - \mu_1) \\ Q_2(\mathrm{x}_1, \mathrm{x}_2) \triangleq \left[(\mathrm{x}_2 - \mu_2) - \Sigma_{12}^T \Sigma_{11}^{-1} (\mathrm{x}_1 - \mu_1)\right]^T \left(\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}\right)^{-} \\ = (\mathrm{x}_2 - b)^T A^{-1} (\mathrm{x}_2 - b) \end{cases}$$

and get

$$Q(\mathbf{x}_1, \mathbf{x}_2) = Q_1(\mathbf{x}_1) + Q_2(\mathbf{x}_1, \mathbf{x}_2)$$

Marginalisation and Conditional of multivariate normal

Now the joint distribution can be written as:

$$
\begin{aligned}
f(\mathrm{x}) = f\left(\mathrm{x}_1, \mathrm{x}_2\right) &= \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left[-\frac{1}{2} Q\left(\mathrm{x}_1, \mathrm{x}_2\right)\right] \\
&= \frac{1}{(2\pi)^{n/2}\left|\Sigma_{11}\right|^{1/2}\left|\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}\right|^{1/2}} \exp\left[-\frac{1}{2} Q\left(\mathrm{x}_1, \mathrm{x}_2\right)\right] \\
&= \frac{1}{(2\pi)^{p/2}\left|\Sigma_{11}\right|^{1/2}} \exp\left[-\frac{1}{2}\left(\mathrm{x}_1 - \mu_1\right)^T \Sigma_{11}^{-1}\left(\mathrm{x}_1 - \mu_1\right)\right] \frac{1}{(2\pi)^{q/2}|A|^{1/}} \\
&= N\left(\mathrm{x}_1, \mu_1, \Sigma_{11}\right) N\left(\mathrm{x}_2, b, A\right)
\end{aligned}
$$

The third equal sign is due to Determinant of a partitioned symmetric matrix:

$$|\Sigma| = \left|\Sigma_{11}\right|\left|\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}\right|$$

Marginalisation and Conditional of multivariate normal

The marginal distribution of $\mathbf{x}_1$ is

$$f_1(\mathbf{x}_1) = \int f(\mathbf{x}_1, \mathbf{x}_2)\, d\mathbf{x}_2 = \frac{1}{(2\pi)^{p/2}\left|\Sigma_{11}\right|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}_1 - \mu_1)^T \Sigma_{11}^{-1} (\mathbf{x}_1$$

and the conditional distribution of $\mathbf{x}_2$ given $\mathbf{x}_1$ is

$$f_{2|1}(\mathrm{x}_2|\mathrm{x}_1) = \frac{f(\mathrm{x}_1, \mathrm{x}_2)}{f(\mathrm{x}_1)} = \frac{1}{(2\pi)^{q/2}|A|^{1/2}} \exp\left[-\frac{1}{2}(\mathrm{x}_2 - b)^T A^{-1} (\mathrm{x}_2 - b)\right.$$

Marginalisation and Conditional of multivariate normal

with

$$b = \mu_2 + \Sigma_{12}^T \Sigma_{11}^{-1} (\mathbf{x}_1 - \mu_1)$$

$$A = \Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}$$